Fermi liquid theory for the nonequilibrium Kondo effect at low bias voltages

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In this report, we describe a recent development in a Fermi liquid theory for the Kondo effect in quantum dots under a finite bias voltage V. Applying the microscopic theory of Yamada and Yosida to a nonequilibrium steady state, we derive the Ward identities for the Keldysh Green's function, and determine the low-energy behavior of the differential conductance dI/dV exactly up to terms of order $(eV)^2$ for the symmetric Anderson model. These results are deduced from the fact that the Green's function at the impurity site is a functional of a nonequilibrium distribution $f_{\rm eff}(\omega)$, which at $eV = 0$ coincides with the Fermi function. Furthermore, we provide an alternative description of the low-energy properties using a renormalized perturbation theory (RPT). In the nonequilibrium state the unperturbed part of the RPT is determined by the renormalized free quasiparticles, the distribution function of which is given by $f_{\rm eff}(\omega)$. The residual interaction between the quasiparticles $\widetilde{U}$, which is defined by the full vertex part at zero frequencies, is taken into account by an expansion in the power series of $\widetilde{U}$. We also discuss the application of the RPT to a high-bias region beyond the Fermi-liquid regime.

KEYWORDS: Kondo effect, Fermi liquid, Nonequilibrium, Keldysh formalism, Anderson model, Quantum dot

1. Introduction

The Kondo effect[1] in quantum dots has been an active research field over a decade. The early prediction about a characteristic gate-voltage dependence of the linear-response conductance[2–4] has been confirmed experimentally in semiconductor devices,[5–8] and other new features of the Kondo physics are also being studied extensively in various situations, such as an AB ring, Josephson junction, ferromagnetic leads, etc.

The equilibrium and linear-response properties of a single quantum dot connected to normal leads can be explained basically based on the knowledge of the Kondo problem in dilute magnetic alloys,[9] although there exists some differences in experimental geometry (configuration) between the impurity in magnetic alloys and quantum dots in semiconductor devices. Therefore, the low-energy properties can be described by the local Fermi liquid theory,[10–12] and the nonperturbative approaches developed for the alloys, such as the quantum Monte Carlo[13,14] and numerical renormalization group (NRG) methods,[15] can be applicable to the quantum dots. Particularly, the NRG has been used successfully to calculate the linear-response conductance of the quantum dots.[15]

The nonlinear transport under a finite bias voltage V, however, is still not fully understood, despite of a number of theoretical efforts.[16–24] Among a variety of aspects of the nonequilibrium properties, in this report we focus our attention mainly on the low-energy properties. Specifically, we describe the Fermi-liquid behavior of the first nonlinear term of the differential conductance dI/dV using the Ward identities, which is derived by applying the perturbation theory in the Coulomb interaction U of Yamada and Yosida to the Keldysh Green's function. We show that the low-energy asymptotic form of the order U^2 self-energy[17] is essentially retained in all orders in U, and the contributions of the higher-order terms are absorbed into the coefficients which can be written in terms of the *local-Fermi-liquid* parameters such as the width of the Kondo resonance $\widetilde{\Delta}$ and Wilson ratio R.[22] The proof was provided previously in ref. 22. In the present report, however, we give another derivation, using the property of the impurity Green's function $\boldsymbol{G}(\omega)$ as a functional of a nonequilibrium distribution function $f_{\rm eff}(\omega)$, through which the dependence of $\boldsymbol{G}(\omega)$ on eV and T arises. This property also allows us to deduce some exact results in the limit of large eV.[23] In the present report, we re-examine the low-energy properties with an emphasis on this aspect of the Green's function as a functional.

We also present an alternative description of the low-voltage Fermi-liquid behavior using the renormalized perturbation theory (RPT).[25] The unperturbed Green's function of the RPT in the Keldysh formalism consists of the propagators of the free quasiparticles, which are determined by the renormalized resonance of the width $\widetilde{\Delta}$ and the nonequilibrium distribution $f_{\rm eff}(\omega)$. To second order in the residual interaction $\widetilde{U}$, which is defined in eq. (44), it gives the exact low-energy $(eV)^2$ coefficient of dI/dV. The higher order terms in $\widetilde{U}$ determine the high-energy properties. It has recently been confirmed that in equilibrium a combination of the RPT and NRG gives an efficient way of calculating the temperature dependence of the susceptibility,[26] so that the RPT seems to be one possible approach to the nonequilibrium properties beyond the Fermi-liquid regime.

In §2, we describe the Keldysh formalism for the Anderson impurity in order to describe clearly the properties of $\boldsymbol{G}(\omega)$ as a functional of $f_{\rm eff}(\omega)$. In §3, we consider the low-energy behavior of the self-energy at small eV using the Ward identities, and give an exact low-energy expression of dI/dV in the electron-hole symmetric case. In §4, the RPT is applied to the low-voltage Fermi-liquid regime, and the procedure of the perturbation expansion

in $\widetilde{U}$ in the Keldysh formalism is provided. In the appendix, details of the Ward identities and properties of $\boldsymbol{G}(\omega)$ as a functional of $f_{\rm eff}(\omega)$ are given.

2. Keldysh Formalism for the Anderson Model

We start with the single Anderson impurity connected to two leads at the left (L) and right (R):

$$H \;=\; H_c \,+\, H_d \,+\, H_{\rm mix} \,+\, H_U \;, \tag{1}$$

$$H_c = \sum_{\lambda=L,R} \sum_{k\sigma} \epsilon_{k\lambda}\, c^\dagger_{k\lambda\sigma} c_{k\lambda\sigma} \,, \tag{2}$$

$$H_d = \sum_\sigma E_d\, n_{d\sigma} \;, \quad H_U = \frac{U}{2}\Big(\sum_\sigma n_{d\sigma} - 1\Big)^2 \;, \tag{3}$$

$$H_{\rm mix} \;=\; \sum_{\lambda=L,R} \sum_{\sigma} v_\lambda \left(d^\dagger_\sigma \psi_{\lambda\sigma} + \psi^\dagger_{\lambda\sigma} d_\sigma \right), \tag{4}$$

where d_σ annihilates an electron with spin σ at the dot, $n_{d\sigma} = d^\dagger_\sigma d_\sigma$, and $E_d = \epsilon_d + U/2$. We assume that the onsite potential ϵ_d is a constant independent of the bias voltage, and take the Fermi level at equilibrium μ to be the origin of the energy, i.e., $\mu = 0$. In the lead at λ ($= L,\, R$), the energy spectrum is given by $\epsilon_{k\lambda} = \epsilon_k + eV_\lambda$. To specify how the bias voltage V is applied to each of the leads, we introduce a parameter α_λ such that $V_L = \alpha_L V$ and $V_R = -\alpha_R V$ with $\alpha_L + \alpha_R = 1$. In eq. (4), v_λ is the tunneling matrix element between the dot and lead at λ, and $\psi_{\lambda\sigma} = \sum_k c_{k\lambda\sigma}/\sqrt{N}$. We will use units $\hbar = 1$.

In the thermal equilibrium, we know that the density matrix is given by $\rho_{\rm eq} \propto {\rm e}^{-\beta H}$, and thus the Hamiltonian determines both the time evolution and statistical weight. However, in a nonequilibrium steady state the density matrix cannot be determined simply by H, and it depends on how the system has been driven to the steady state. The Keldysh formalism has been used widely for this purpose to determine the density matrix $\widehat{\rho}(t)$ for nonequilibrium states.[27–29]

The method uses the procedure of an adiabatic switching on, which is described by the operator $\mathcal{U}(t,t_0) = {\rm T}\exp[\,-{\rm i}\int_{t_0}^t {\rm d}t'\,\widetilde{H}_2(t')\,]$. Here, $\widetilde{O}(t) \equiv {\rm e}^{{\rm i}H_1 t} O\, {\rm e}^{-{\rm i}H_1 t}$ is an operator in the interaction representation with respect to H_1, which is a time-independent part of the total Hamiltonian $H(t) = H_1 + H_2\, {\rm e}^{-\delta|t|}$. In the interaction representation the density matrix defined by $\widetilde{\rho}(t) \equiv {\rm e}^{{\rm i}H_1 t}\, \widehat{\rho}(t)\, {\rm e}^{-{\rm i}H_1 t}$ can be rewritten in the form

$$\widetilde{\rho}(t) \;=\; \mathcal{U}(t,-\infty)\, \widetilde{\rho}(-\infty)\, \mathcal{U}(-\infty,t) \;, \tag{5}$$

where $\widetilde{\rho}(-\infty)$ represents the initial statistical weight. The average value of a Heisenberg operator $\mathcal{O}_H(t) = \mathcal{U}(0,t)\, \widetilde{\mathcal{O}}(t)\, \mathcal{U}(t,0)$ is given by

$$\begin{aligned} \langle \mathcal{O}_H(t) \rangle \;&\equiv\; {\rm Tr}\,[\,\widehat{\rho}(0)\, \mathcal{O}_H(t)\,] \\ &= {\rm Tr}\Big[\,\widetilde{\rho}(-\infty)\, \mathcal{U}(-\infty,+\infty)\, \mathcal{U}(+\infty,t)\, \widetilde{\mathcal{O}}(t)\, \mathcal{U}(t,-\infty)\,\Big] . \end{aligned} \tag{6}$$

The stream of time seen in this expression is usually illustrated as the Keldysh contour shown in Fig. 1: the + branch corresponds to the time evolution by the operator $\mathcal{U}(-\infty,+\infty) = \widetilde{\rm T}\exp[\,{\rm i}\int_{-\infty}^{\infty} {\rm d}t'\,\widetilde{H}_2(t')\,]$, where $\widetilde{\rm T}$ denotes the anti-time-ordering operator. If one chooses

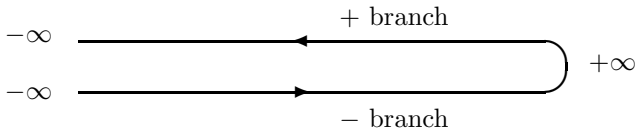

Fig. 1. The Keldysh contour for the time evolution.

H_1 to be bilinear, the Feynman-diagrammatic approach is applicable for the Green's functions defined by

$$G^{--}_\sigma(t) \;=\; -{\rm i}\,\langle {\rm T}\, d_\sigma(t)\, d^\dagger_\sigma(0)\rangle \;, \tag{7}$$

$$G^{-+}_\sigma(t) \;=\; {\rm i}\,\langle d^\dagger_\sigma(0)\, d_\sigma(t)\rangle \;, \tag{8}$$

$$G^{+-}_\sigma(t) \;=\; -{\rm i}\,\langle d_\sigma(t)\, d^\dagger_\sigma(0)\rangle \;, \tag{9}$$

$$G^{++}_\sigma(t) \;=\; -{\rm i}\,\langle \widetilde{\rm T}\, d_\sigma(t)\, d^\dagger_\sigma(0)\rangle \;. \tag{10}$$

These functions are linearly dependent $G^{-+} + G^{+-} = G^{--} + G^{++}$. Furthermore, the retarded and advanced Green's functions can be written as $G^r = G^{--} - G^{-+}$ and $G^a = G^{--} - G^{+-}$, respectively.

2.1 Traditional Formulation

To describe a nonequilibrium steady state under a finite bias voltage, Caroli *et al.*[28] has introduced the initial statistical weight of the form

$$\widetilde{\rho}(-\infty) \,\propto\, {\rm e}^{-\beta(\,H_d\,+\,H_c\,-\,\mu_L N_L\,-\,\mu_R N_R\,)} \;, \tag{11}$$

where $N_\lambda = \sum_{k\sigma} c^\dagger_{k\lambda\sigma} c_{k\lambda\sigma}$. The two chemical potentials, $\mu_L \equiv eV_L$ and $\mu_R \equiv eV_R$, are defined with respect to the isolated systems described by $H_1 = H_d + H_c$, and the remaining part $H_2 = H_{\rm mix} + H_U$ is switched on adiabatically. Specifically, in the noninteracting case $U = 0$, the Green's functions can be written in the form

$$G^{--}_0(\omega) = [1 - f_{\rm eff}(\omega)]\, G^r_0(\omega) \,+\, f_{\rm eff}(\omega)\, G^a_0(\omega) \;, \tag{12}$$

$$G^{-+}_0(\omega) \;=\; -\,f_{\rm eff}(\omega)\,[\,G^r_0(\omega) - G^a_0(\omega)\,] \,, \tag{13}$$

$$G^{+-}_0(\omega) \;=\; [1 - f_{\rm eff}(\omega)]\,[\,G^r_0(\omega) - G^a_0(\omega)\,] \,, \tag{14}$$

$$G^{++}_0(\omega) \;=\; -\,[1 - f_{\rm eff}(\omega)]\, G^a_0(\omega) \,-\, f_{\rm eff}(\omega)\, G^r_0(\omega), \tag{15}$$

where $G^r_0(\omega) = \big[\,\omega - E_d + {\rm i}\Delta\,\big]^{-1}$, $G^a(\omega) = \{G^r(\omega)\}^*$, and $\Delta = \Gamma_L + \Gamma_R$ with $\Gamma_\lambda = \pi\rho_\lambda v_\lambda^2$. We assume that the density of states $\rho_\lambda(\omega) = \sum_k \delta(\omega - \epsilon_{k\lambda})/N$ is a constant, and the band width is very large. One important feature we see in eqs. (12)–(15) is that all the information about the nonequilibrium distribution is contained in the distribution function,[17]

$$f_{\rm eff}(\omega) \;=\; \frac{f_L(\omega)\,\Gamma_L + f_R(\omega)\,\Gamma_R}{\Gamma_L + \Gamma_R} \;. \tag{16}$$

Here $f_\lambda(\omega) = f(\omega - \mu_\lambda)$, and $f(\omega) = [\,{\rm e}^{\omega/T} + 1\,]^{-1}$. At $T = 0$ the distribution function $f_{\rm eff}(\omega)$ has two steps, at $\omega = \mu_L$ and μ_R, as shown in Fig. 2. At $eV = 0$, it coincides with the usual Fermi function $f(\omega)$.

The interacting Green's function $\boldsymbol{G}(\omega)$ satisfies the Dyson equation,

$$\{\boldsymbol{G}(\omega)\}^{-1} = \{\boldsymbol{G}_0(\omega)\}^{-1} - \boldsymbol{\Sigma}(\omega) \;, \tag{17}$$

$$\boldsymbol{G}_0 \;=\; \begin{bmatrix} G^{--}_0 & G^{-+}_0 \\ G^{+-}_0 & G^{++}_0 \end{bmatrix}, \quad \boldsymbol{\Sigma} = \begin{bmatrix} \Sigma^{--} & \Sigma^{-+} \\ \Sigma^{+-} & \Sigma^{++} \end{bmatrix}. \tag{18}$$

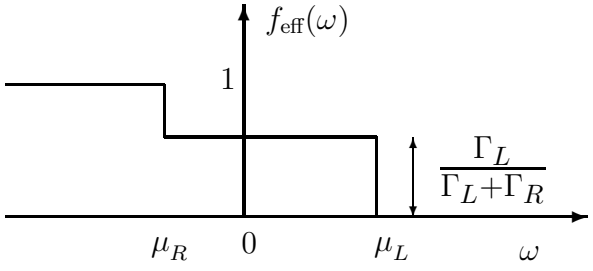

Fig. 2. The nonequilibrium distribution $f_{\rm eff}(\omega)$ at $T=0$.

Here $\mathbf{\Sigma}(\omega)$ is the self-energy due to H_U: the four elements are linearly dependent $\Sigma^{-+}+\Sigma^{+-} = -\Sigma^{--}-\Sigma^{++}$, and we have also two extra relations in the ω-space, $\Sigma^a(\omega) = \{\Sigma^r(\omega)\}^*$ and $\Sigma^{--}(\omega) = -\{\Sigma^{++}(\omega)\}^*$. Using these relations, the retarded Green's function is written in the form

$$G^r(\omega) \;=\; \frac{1}{\omega - E_d + {\rm i}\Delta - \Sigma^r(\omega)} \tag{19}$$

with $\Sigma^r = \Sigma^{--}+\Sigma^{-+}$. The four elements of $\boldsymbol{G}(\omega)$ are also written in the forms similar to eqs. (12)–(15), for which G_0^r and G_0^a are replaced by the interacting ones and $f_{\rm eff}(\omega)$ is replaced by a correlated distribution defined by

$$f_{\rm eff}^U(\omega) = \frac{f_L(\omega)\,\Gamma_L + f_R(\omega)\,\Gamma_R - \dfrac{1}{2{\rm i}}\,\Sigma^{-+}(\omega)}{\Gamma_L+\Gamma_R - {\rm Im}\Sigma^r(\omega)}\;. \tag{20}$$

This function was introduced by Hershfield *et al.*, and was studied using the order U^2 self-energy.[17] Note that $\Sigma^{-+}(\omega)$ is pure imaginary, and at $eV=0$ it takes the form $\Sigma^{-+}(\omega)|_{eV=0} = 2{\rm i}f(\omega){\rm Im}\,\Sigma^r(\omega)|_{eV=0}$. Thus, in the nonequilibrium state, the distribution function $f_{\rm eff}^U(\omega)$ generally depends on the interaction U, while in equilibrium $eV=0$ it coincides with the Fermi function.

2.2 Alternative Formulation

As described in the above, the noninteracting Green's function for $H_0 \equiv H_c + H_d + H_{\rm mix}$ can be calculated analytically taking all contributions of the tunneling matrix element $H_{\rm mix}$ into account. A question arises: do we always have to start with the isolated systems to obtain eqs. (12)–(15)? The answer is no. An alternative description was given by Hershfield.[30] The basic idea is to assign the two different chemical potentials directly to the left- and right-moving scattering states which are written formally, using the Lippmann-Schwinger equation, as

$$\gamma_{k\lambda\sigma}^\dagger \;=\; c_{k\lambda\sigma}^\dagger \;+\; \frac{1}{\varepsilon_k - H_0 + {\rm i}\delta}\,H_{\rm mix}\,c_{k\lambda\sigma}^\dagger\;, \tag{21}$$

where $\lambda = L,\,R$. The incident wave comes in the left for $\gamma_{kL\sigma}^\dagger$, and in the right for $\gamma_{kR\sigma}^\dagger$. These scattering states are the eigenstates, by which H_0 can be diagonalized as

$$H_0 \;=\; \sum_{\lambda=L,R}\sum_{k\sigma}\varepsilon_k\gamma_{k\lambda\sigma}^\dagger\gamma_{k\lambda\sigma}\;. \tag{22}$$

Note that generally the bound states and continuum states without the degeneracy (for the left and right movers) are present. Such states are not distinguished from the degenerate scattering states in eq. (22) for simplicity. With these scattering states, the density matrix for $U=0$ can be expressed explicitly as[30]

$$\widehat{\rho}_0(0) \;\propto\; {\rm e}^{-\beta(\,H_d + H_c + H_{\rm mix} - \mu_L\mathcal{N}_L - \mu_R\mathcal{N}_R\,)}\;, \tag{23}$$

where $\mathcal{N}_{\lambda\sigma} = \sum_k \gamma_{k\lambda\sigma}^\dagger\gamma_{k\lambda\sigma}$. One can confirm that the noninteracting Green's functions eqs. (12)–(15) can be calculated directly from eq. (23). Therefore, the Coulomb interaction H_U can be switched on starting from the connected system taking $\widehat{\rho}_0(0)$, given in eq. (23), to be the initial statistical weight. It is carried out by using eq. (6) and redefining the initial condition as $H_1 \Rightarrow H_0$, $H_2 \Rightarrow H_U$, and $\widetilde{\rho}(-\infty) \Rightarrow {\rm e}^{-\beta(\,H_0 - \mu_L\mathcal{N}_L - \mu_R\mathcal{N}_R\,)}$.

The perturbation series in U of the nonequilibrium Green's function $\boldsymbol{G}$ can be generated automatically using the path integral representation,[31]

$$\mathcal{Z} \;=\; \int\mathcal{D}\eta^\dagger\mathcal{D}\eta\;{\rm e}^{{\rm i}S}\;, \tag{24}$$

$$G_\sigma^{\nu\nu'}(t,t') \;=\; \frac{-{\rm i}}{\mathcal{Z}}\int\mathcal{D}\eta^\dagger\mathcal{D}\eta\;{\rm e}^{{\rm i}S}\,\eta_{\sigma\nu}(t)\,\eta_{\sigma\nu'}^\dagger(t')\;, \tag{25}$$

where $\eta_{\sigma\nu}(t)$ is a Grassmann number for the branch ν $(=-,\,+)$ in the Keldysh contour. The action S is defined by

$$S \;=\; S_0 \;+\; S_U\;, \tag{26}$$

$$S_0 \;=\; \sum_\sigma\int_{-\infty}^{\infty}{\rm d}t\,{\rm d}t'\;\boldsymbol{\eta}_\sigma^\dagger(t)\,\boldsymbol{K}_0(t,t')\,\boldsymbol{\eta}_\sigma(t')\;, \tag{27}$$

$$S_U \;=\; -\,\frac{U}{2}\int_{-\infty}^{\infty}{\rm d}t\left[\left(\sum_\sigma\eta_{\sigma-}^\dagger(t)\,\eta_{\sigma-}(t)\;-\;1\right)^2 - \left(\sum_\sigma\eta_{\sigma+}^\dagger(t)\,\eta_{\sigma+}(t)\;-\;1\right)^2\right], \tag{28}$$

where

$$\boldsymbol{K}_0(t,t') \;=\; \int_{-\infty}^{\infty}\frac{{\rm d}\omega}{2\pi}\,\{\boldsymbol{G}_0(\omega)\}^{-1}\,{\rm e}^{-{\rm i}\omega(t-t')}\;, \tag{29}$$

and $\boldsymbol{\eta}_\sigma^\dagger(t) = \big(\,\eta_{\sigma-}^\dagger(t)\,,\,\eta_{\sigma+}^\dagger(t)\,\big)$. In the Keldysh formalism the perturbation expansion works with the real frequencies (or real times). Therefore, eq. (25) shows that the dependence of $\boldsymbol{G}(\omega)$ on the bias voltage and temperature arises through $f_{\rm eff}(\omega)$ in the noninteracting Green's function $\boldsymbol{G}_0(\omega)$ which determines S_0 via eqs. (27) and (29). Thus, the full Green's function $\boldsymbol{G}(\omega)$, can be regarded as a functional of $f_{\rm eff}(\omega)$. The precise form of the functional is obtained by expanding ${\rm e}^{{\rm i}S}$ in eq. (25) in the power series of U, and substituting eqs. (12)–(15) into every single $\boldsymbol{G}_0$'s in the series. Therefore, the change in the self-energy, $\delta\mathbf{\Sigma}$, caused by a small variation in the distribution function, $\delta f_{\rm eff}$, can be expressed in the form

$$\delta\mathbf{\Sigma}_\sigma(\omega) \;=\; \sum_{\nu\nu'\sigma'}\int_{-\infty}^{\infty}{\rm d}\omega'\,\frac{\delta\mathbf{\Sigma}_\sigma(\omega)}{\delta G_{0\sigma'}^{\nu\nu'}(\omega')}\bigg|_{\delta f_{\rm eff}=0}\delta G_{0\sigma'}^{\nu\nu'}(\omega') \;+\; \Big[\,\text{higer order terms in }\delta f_{\rm eff}\,\Big]\;, \tag{30}$$

where

$$\delta G_{0\sigma'}^{\nu\nu'}(\omega') \;=\; -\,[\,G_{0\sigma'}^r(\omega') - G_{0\sigma'}^a(\omega')\,]\;\delta f_{\rm eff}(\omega')\;. \tag{31}$$

The functional derivative $\delta\mathbf{\Sigma}_\sigma/\delta G_{0\sigma'}^{\nu\nu'}$ can be related to

the vertex corrections in the Keldysh formalism. The functional aspect discussed here is analogous to the functional approach of Luttinger and Ward.[32] However, in eq. (30), the functional derivative is taken with respect to noninteracting Green's function. At finite temperatures $T \neq 0$ the distribution function $f_{\rm eff}(\omega)$ dose not have the discontinuities, and thus it can be treated as a regular function in general discussions. Nevertheless, the singularities appearing in the limit of $T \to 0$ play an important role, for instance, as we see in eq. (39).

3. Fermi-Liquid Behavior at Small Voltages

In equilibrium and linear-response regime, the low-energy properties at ω, $T \ll T_K$ can be described by the local Fermi liquid theory,[10] where T_K is the Kondo temperature. The Fermi liquid theory can also describe the nonlinear response at small bias-voltages $eV \ll T_K$.[22] Our proof uses the Ward identities[11,12,33] in the Keldysh formalism. In this section, we describe the outline of the derivation of the identities, and then determine the low-voltage behavior of the differential conductance dI/dV up to terms of order $(eV)^2$ in the electron-hole symmetric case.

3.1 Ward identities

We first of all consider the behavior of $\boldsymbol{G}_0(\omega)$ at small eV. The first derivative at $eV = 0$ is written in the form

$$\left.\frac{\partial G_0^{\nu\nu'}(\omega)}{\partial(eV)}\right|_{eV=0} = -\alpha\left(\frac{\partial}{\partial\omega}+\frac{\partial}{\partial E_d}\right)G_{0:\rm eq}^{\nu\nu'}(\omega)\,, \quad (32)$$

where $\alpha \equiv (\alpha_L\Gamma_L - \alpha_R\Gamma_R)/(\Gamma_L+\Gamma_R)$, and the label "eq" in the subscript stands for the "equilibrium", so that $G_{0:\rm eq}^{\nu\nu'} \equiv G_0^{\nu\nu'}\big|_{eV=0}$. Owing to the properties of $f_{\rm eff}(\omega)$, the differential coefficient with respect to eV can be related to the equilibrium quantities in the right-hand side eq. (32). From the discussions in §2, the self-energy can also be regarded a functional of $\boldsymbol{G}_0(\omega)$. Thus, the differential coefficients of $\boldsymbol{\Sigma}(\omega)$ with respect to eV can be calculated taking the derivative of $\boldsymbol{G}_0$'s appearing in the perturbation series in U, as described in the appendix. Then, using eq. (32), we obtain

$$\left.\frac{\partial\boldsymbol{\Sigma}(\omega)}{\partial(eV)}\right|_{eV=0} = -\alpha\left(\frac{\partial}{\partial\omega}+\frac{\partial}{\partial E_d}\right)\boldsymbol{\Sigma}_{\rm eq}(\omega)\,, \quad (33)$$

$$\left.\frac{\partial^2\boldsymbol{\Sigma}(\omega)}{\partial(eV)^2}\right|_{eV=0} = \alpha^2\left(\frac{\partial}{\partial\omega}+\frac{\partial}{\partial E_d}\right)^2\boldsymbol{\Sigma}_{\rm eq}(\omega) + \frac{\Gamma_L\,\Gamma_R}{(\Gamma_L+\Gamma_R)^2}\,\widehat{D}^2\boldsymbol{\Sigma}_{\rm eq}(\omega)\,, \quad (34)$$

where $\boldsymbol{\Sigma}_{\rm eq}(\omega) \equiv \boldsymbol{\Sigma}(\omega)|_{eV=0}$. The operator $\widehat{D}^2$ acts on the noninteracting Green's functions in the perturbation series for $\boldsymbol{\Sigma}_{\rm eq}(\omega)$, and it takes the second derivative $(\partial/\partial\omega' + \partial/\partial E_d)^2$, as

$$\widehat{D}^2\boldsymbol{\Sigma}_{{\rm eq},\sigma}(\omega) = \sum_{\nu\nu'\sigma'}\int {\rm d}\omega' \frac{\delta\boldsymbol{\Sigma}_{{\rm eq},\sigma}(\omega)}{\delta G_{0:{\rm eq},\sigma'}^{\nu\nu'}(\omega')}\left(\frac{\partial}{\partial\omega'}+\frac{\partial}{\partial E_d}\right)^2 G_{0:{\rm eq},\sigma'}^{\nu\nu'}(\omega'). \quad (35)$$

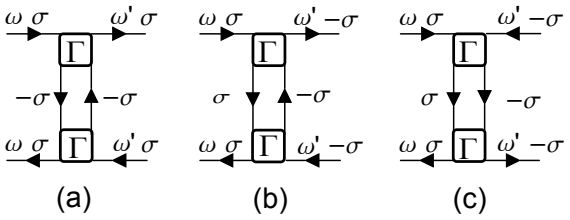

Fig. 3. The diagrams contribute to the singularities.

Using these relations, the low-bias behavior of the self-energy can be deduced from the equilibrium quantities.

Specifically, at $T = 0$ and $eV = 0$, the usual zero-temperature formalism is applicable for the causal Green's function defined with respect to the equilibrium ground state,

$$G_{\rm eq}^{--}(\omega) = G_{\rm eq}^{r}(\omega)\,\theta(\omega) + G_{\rm eq}^{a}(\omega)\,\theta(-\omega)\,, \quad (36)$$

where $\theta(\omega)$ is the Heaviside step function. Thus at $T = 0$ the causal matrix-element in the right-hand side of eq. (33) can be related to the vertex corrections,[33]

$$\left(\frac{\partial}{\partial\omega}+\frac{\partial}{\partial E_d}\right)\Sigma_{{\rm eq},\sigma}^{--}(\omega) = -\sum_{\sigma'}\Gamma_{\sigma\sigma';\sigma'\sigma}(\omega,0;0,\omega)\,A_{{\rm eq},\sigma'}(0)\,, \quad (37)$$

where $\Gamma_{\sigma\sigma';\sigma'\sigma}(\omega,\omega';\omega',\omega)$ is the vertex function for the causal Green's function in the $T = 0$ formalism, and $A_{{\rm eq},\sigma}(\omega) = -{\rm Im}\,G_{{\rm eq},\sigma}^{r}(\omega)/\pi$. Similarly, the causal element of $\widehat{D}^2\boldsymbol{\Sigma}_{{\rm eq},\sigma}$ can be written as[22]

$$\widehat{D}^2\Sigma_{{\rm eq},\sigma}^{--}(\omega) = \sum_{\sigma'}\frac{\partial}{\partial\omega'}\,\Gamma_{\sigma\sigma';\sigma'\sigma}(\omega,\omega';\omega',\omega)\,A_{{\rm eq},\sigma'}(\omega')\Big|_{\omega'=0}\,. \quad (38)$$

Eliashberg[34] has shown quite generally by using the Lehmann representation that the imaginary part of the vertex function has some singularities.[12,33,35] For small frequencies, the singularities relevant to eqs. (37) and (38) arise from the diagrams shown in Fig. 3. The asymptotic form of the imaginary part of eq. (38) at small ω and ω' can be calculated as[22]

$$\begin{aligned}
&\sum_{\sigma'}\frac{\partial}{\partial\omega'}\,{\rm Im}\,\Gamma_{\sigma\sigma';\sigma'\sigma}(\omega,\omega';\omega',\omega)\\
&= -\,|\Gamma_{\uparrow\downarrow;\downarrow\uparrow}(0,0;0,0)|^2\\
&\quad\times{\rm Im}\left[2\int\frac{d\omega''}{2\pi{\rm i}}\,G_{\rm eq}^{--}(\omega'')\,\frac{\partial}{\partial\omega'}G_{\rm eq}^{--}(\omega-\omega'+\omega'')\right.\\
&\qquad\left.+\int\frac{d\omega''}{2\pi{\rm i}}\,G_{\rm eq}^{--}(\omega'')\,\frac{\partial}{\partial\omega'}G_{\rm eq}^{--}(\omega+\omega'-\omega'')\right]\\
&= -\,\pi\,\{A_{\rm eq}(0)\}^2\,|\Gamma_{\uparrow\downarrow;\downarrow\uparrow}(0,0;0,0)|^2\\
&\quad\times\Big[-2\,{\rm sgn}(\omega'-\omega)\,+\,{\rm sgn}(\omega'+\omega)\Big]\,. \qquad (39)
\end{aligned}$$

Here the first term in the last line corresponds to the contributions of the diagram (a) and (b), and the second term corresponds to that of the diagram (c). Due to these

singularities, the value of eq. (39) in the limit of $\omega, \omega' \to 0$ depends on which frequency is taken first to be zero. Taking the limit for small frequencies carefully, the low-energy behavior of $\mathrm{Im}\,\Sigma^r(\omega)$ are determined up to terms of order ω^2, $(eV)^2$, and T^2,

$$\mathrm{Im}\,\Sigma^r(\omega) = -\frac{\pi}{2}\{A_{\rm eq}(0)\}^3\,|\Gamma_{\uparrow\downarrow;\downarrow\uparrow}(0,0;0,0)|^2 \times\left[(\omega-\alpha\,eV)^2+\frac{3\,\Gamma_L\Gamma_R}{(\Gamma_L+\Gamma_R)^2}(eV)^2+(\pi T)^2\right]. \quad (40)$$

The result at equilibrium $eV = 0$ has been provided by Yamada and Yosida,[11] and it is extended to the nonequilibrium steady state here up to terms of order $(eV)^2$. Note that we have not assumed the electron-hole symmetry so far.

3.2 Results in the electron-hole symmetric case

In this subsection we consider the low-energy behavior of $G^r(\omega)$ and dI/dV using the result of $\mathrm{Im}\,\Sigma^r(\omega)$ obtained in eq. (40). Specifically, we concentrate on the electron-hole symmetric case, where $\epsilon_d = -U/2$, $\Gamma_L = \Gamma_R$, and $\alpha_L = \alpha_R = 1/2$. In this case $A_{\rm eq}(0) = 1/(\pi\Delta)$, and the real part of the self-energy takes the form

$$\mathrm{Re}\,\Sigma^r(\omega) = \left(1-z^{-1}\right)\omega + O(\omega^3)\,, \quad (41)$$

$$z \equiv \left(1-\left.\frac{\partial\Sigma^r_{\rm eq}(\omega)}{\partial\omega}\right|_{\omega=0}\right)^{-1}. \quad (42)$$

Thus, $G^r(\omega)$ can be calculated exactly up to terms of order ω^2, T^2 and $(eV)^2$ using eq. (40),

$$G^r(\omega) \simeq \frac{z}{\omega+\mathrm{i}\,\widetilde{\Delta}+\mathrm{i}\,\dfrac{\widetilde{U}^2}{2\widetilde{\Delta}(\pi\widetilde{\Delta})^2}\left[\omega^2+\dfrac{3}{4}(eV)^2+(\pi T)^2\right]}, \quad (43)$$

where the renormalized parameters are defined by

$$\widetilde{\Delta} \equiv z\Delta\,, \qquad \widetilde{U} \equiv z^2\,\Gamma_{\uparrow\downarrow;\downarrow\uparrow}(0,0;0,0)\,. \quad (44)$$

The order U^2 result of Hershfield *et al.*[17] can be reproduced from eq. (43) replacing $\widetilde{U}$ by the bare Coulomb interaction U, and using the order U^2 result for the renormalization factor[11,36] $z = 1-(3-\pi^2/4)\,u^2+\cdots$, where $u = U/(\pi\Delta)$.

Thus, in the symmetric case the low-voltage behavior is characterized by the two parameters $\widetilde{\Delta}$ and $\widetilde{U}$. These parameters are defined with respect to the equilibrium ground state, for which the exact Bethe ansatz results exist[36–38] as shown in Fig. 4. The width of the Kondo resonance $\widetilde{\Delta}$ decreases with increasing U, and for $u \gtrsim 2.0$ it is approximated well by the asymptotic form $\widetilde{\Delta} \simeq (4/\pi)T_K$, where the Kondo temperature is defined by

$$T_K = \pi\Delta\sqrt{u/(2\pi)}\,\exp[-\pi^2u/8+1/(2u)]\,. \quad (45)$$

The Wilson ratio is usually defined by $R \equiv \widetilde{\chi}_s/\widetilde{\gamma}$, where $\widetilde{\gamma}$ and $\widetilde{\chi}_s$ are the enhancement factors for the T-linear specific heat and spin susceptibility, respectively.[11] Alternatively, it can be written in terms of $\widetilde{\Delta}$ and $\widetilde{U}$, as[25]

$$R-1 = \widetilde{U}/(\pi\widetilde{\Delta})\,. \quad (46)$$

The Wilson ratio increases with u from the noninteracting value $R = 1$ to the strong-coupling limit value $R = 2$. The charge excitations at the impurity site are still surviving for $u \lesssim 2.0$, and it makes the value of R smaller than 2.

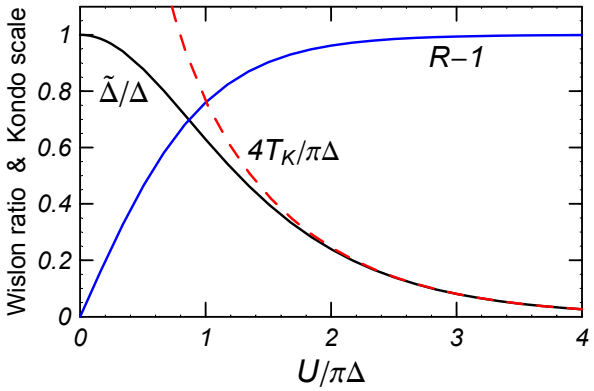

Fig. 4. The U dependence of $\widetilde{\Delta}/\Delta$ and $R-1$, which can also be interpreted as z and $\widetilde{U}/(\pi\widetilde{\Delta})$, respectively. These parameters were calculated using the Bethe ansatz solution summarized in ref. 36.

The nonequilibrium current I can be calculated from the retarded Green's function,[39]

$$I = \frac{2e}{h}\int_{-\infty}^{\infty}\mathrm{d}\omega\,[\,f_L-f_R\,]\,\frac{4\,\Gamma_L\Gamma_R}{\Gamma_R+\Gamma_L}\,[\,-\mathrm{Im}\,G^r(\omega)\,]\,. \quad (47)$$

Substituting eq. (43) into eq. (47), the differential conductance dI/dV can be determined exactly up to terms of order T^2 and $(eV)^2$,

$$\frac{dI}{dV} = \frac{2e^2}{h}\left[1-\frac{1+2\,(R-1)^2}{3}\left(\frac{\pi T}{\widetilde{\Delta}}\right)^2 - \frac{1+5\,(R-1)^2}{4}\left(\frac{eV}{\widetilde{\Delta}}\right)^2+\cdots\right]. \quad (48)$$

The result shows that the nonlinear $(eV)^2$ term is also scaled by the resonance width $\widetilde{\Delta}$, and the coefficient generally depends on the parameter $(R-1)^2$, or $\widetilde{U}^2/(\pi\widetilde{\Delta})^2$. As mentioned, in the strong-coupling limit $u \to \infty$, the two characteristic parameters become $\widetilde{\Delta} \to (4/\pi)\,T_K$ and $R \to 2$.

3.3 Comparison with other approaches

To our knowledge, similar attempts to calculate the coefficient c_V of the $(eV)^2$ term of dI/dV have been made by two groups[20,21] in the strong-coupling limit $u \to \infty$:

$$\frac{dI}{dV} = \frac{2e^2}{h}\left[1-c_T\left(\frac{\pi T}{T_K}\right)^2-c_V\left(\frac{eV}{T_K}\right)^2+\cdots\right]. \quad (49)$$

To compare the results, the difference in a numerical factor of order 1 in the definition T_K must be taken into account. To avoid this uncertainty, we use T_K defined in eq. (45), and rescale the results presented in refs. 20 and 21 such that the coefficient for the linear-response T^2 term agrees with the result of Yamada and Yosida $c_T = (\pi/4)^2$. Kaminski, Nazarov, and Glazman[20]

have carried out a perturbation expansion around the strong-coupling fixed point to obtain $c_V^{\rm KNG} = (3/8)\, c_T$. Konik, Saleur, and Ludwig[21] have used the equilibrium Bethe ansatz solution, and then made some extra assumptions for calculating the nonlinear coefficient to obtain $c_V^{\rm KSL} = 4\, c_T$ (the parameters corresponding to α_L and α_R used by KSL seem to be different from ours). Our result eq. (48), which is obtained using the Ward identities, shows $c_V^{\rm Ward} = (3/2)\, c_T$ in the strong-coupling limit.

Although the Hamiltonian is somewhat different, we also note for comparison that Schiller and Hershfield[19] obtained the result corresponding to $c_V^{\rm SH} = 3\, c_T$ for a special parameter set which can be related to the Emery-Kivelson solution of the two-channel Kondo model.

4. Renormalized Perturbation Theory at Finite Bias Voltages

Although the description of the low-energy properties discussed in §3 is exact, the underlying physics of the quasiparticles might not be seen directly in the microscopic derivation. In the case of the three-dimensional Fermi liquid, the vertex function played a central role to clarify a link between the intuitive picture of the quasiparticles and Green's functions. Specifically, the residual interaction between two quasiparticles, which had been introduced phenomenologically, was shown to be connected to the forward scattering amplitude.[40]

For the Anderson impurity the vertex function at Fermi energy, $z^2\Gamma_{\uparrow\downarrow;\downarrow\uparrow}(0,0;0,0)$, corresponds to the scatter amplitude, and it is equal to $\widetilde{U}$ by the definition in eq. (44). The perturbation expansion in $\widetilde{U}$, which has been formulated precisely in the equilibrium case by Hewson,[25] provides the link between the quasiparticles and microscopic theory of the local Fermi liquid. All the basic Fermi-liquid behavior have been shown to be reproduced in the expansion up to terms of order $\widetilde{U}^2$. Furthermore, the approach is not limited to low energies. To carry out the expansion systematically, however, one has to take account of the renormalization conditions that are necessary to avoid overcounting of the many-body effects, because in the renormalized perturbation theory (RPT) the expansion parameter already contains some contributions of the Coulomb interaction.

In this section we apply the RPT to the nonequilibrium steady state. It reproduces the result of dI/dV in the Fermi-liquid regime, and gives us one possible way to calculate the corrections needed at high voltages. For simplicity, we concentrate on the electron-hole symmetric case; $\epsilon_d = -U/2$, $\Gamma_L = \Gamma_R$, and $\alpha_L = \alpha_R = 1/2$. The unperturbed Green's function is defined such that it describes the Kondo resonance with the renormalized level width $\widetilde{G}_0^r(\omega) = \big[\omega + {\rm i}\widetilde{\Delta}\big]^{-1}$, as that in the equilibrium case.[25] However, in the nonequilibrium case, it is not obvious how the distribution function for the free quasiparticles should be given by. We simply assume here that it is given by the noninteracting one, which in the electron-hole symmetric case takes the form $f_{\rm eff}(\omega) = [\, f(\omega - eV/2) + f(\omega + eV/2)\,]/2$. Hence, the four elements of the unperturbed Green's functions, $\widetilde{\boldsymbol{G}}_0$, take the forms

$$\widetilde{G}_0^{--}(\omega) = \big[1 - f_{\rm eff}(\omega)\big]\, \widetilde{G}_0^r(\omega) + f_{\rm eff}(\omega)\, \widetilde{G}_0^a(\omega), \tag{50}$$

$$\widetilde{G}_0^{-+}(\omega) = -\, f_{\rm eff}(\omega)\, \Big[\, \widetilde{G}_0^r(\omega) - \widetilde{G}_0^a(\omega)\, \Big]\,, \tag{51}$$

$$\widetilde{G}_0^{+-}(\omega) = \big[1 - f_{\rm eff}(\omega)\big]\, \Big[\, \widetilde{G}_0^r(\omega) - \widetilde{G}_0^a(\omega)\, \Big]\,, \tag{52}$$

$$\widetilde{G}_0^{++}(\omega) = -\big[1 - f_{\rm eff}(\omega)\big]\, \widetilde{G}_0^a(\omega) - f_{\rm eff}(\omega)\, \widetilde{G}_0^r(\omega)\,. \tag{53}$$

Correspondingly, the full propagator of the quasiparticles, which includes all effects of $\widetilde{U}$, is defined by $\widetilde{\boldsymbol{G}}(\omega) \equiv z^{-1}\boldsymbol{G}(\omega)$. Therefore, in terms of the renormalized quantities, the nonequilibrium current, eq. (47), is written as

$$I \,=\, \frac{2e}{h} \int_{-\infty}^{\infty} {\rm d}\omega\, [\, f_L - f_R\,] \Big[-\, \widetilde{\Delta}\, {\rm Im}\, \widetilde{G}^r(\omega) \Big]\,. \tag{54}$$

The self-energy correction due to $\widetilde{U}$ satisfies the Dyson equation of the form $\widetilde{\boldsymbol{\Sigma}}(\omega) \,\equiv\, \{\widetilde{\boldsymbol{G}}_0(\omega)\}^{-1} - \{\widetilde{\boldsymbol{G}}(\omega)\}^{-1}$. Using eq. (17), we have

$$\begin{aligned} \widetilde{\boldsymbol{\Sigma}}(\omega) \;&= \{\widetilde{\boldsymbol{G}}_0(\omega)\}^{-1} \,-\, z\, \big[\, \{\boldsymbol{G}_0(\omega)\}^{-1} - \boldsymbol{\Sigma}(\omega)\,\big] \\ &= z\, \boldsymbol{\Sigma}(\omega) \,+\, (1-z)\boldsymbol{\tau}_3\, \omega\,, \end{aligned} \tag{55}$$

where $\boldsymbol{\tau}_i$ for $i = 1, 2, 3$ is the Pauli matrix.

4.1 *Low-energy behavior up to terms of order ω^2, T^2 and $(eV)^2$*

At low-energies, the ω-linear contributions in the right-hand side of eq. (55) cancel out owing to eq. (41). The contributions of order ω^2, T^2 and $(eV)^2$ arise from the second-order diagram for $\widetilde{\boldsymbol{\Sigma}}(\omega)$ shown in Fig. 5, where the solid and dotted lines represent $\widetilde{\boldsymbol{G}}_0(\omega)$ and $\widetilde{U}$, respectively. Calculating the contributions from the diagram, and then taking the cancellation of the ω-linear term into account, we have

$$\widetilde{\Sigma}^r(\omega) \,=\, -\,{\rm i}\, \frac{\widetilde{U}^2}{2\widetilde{\Delta}(\pi\widetilde{\Delta})^2} \left[\omega^2 + \frac{3}{4}\,(eV)^2 + (\pi T)^2 \right] \,+\, \cdots\,. \tag{56}$$

It simply reproduces the renormalized Green's function $\widetilde{G}^r(\omega)$ corresponding to eq. (43). Furthermore, using eq. (54), the $(eV)^2$ term of dI/dV in eq. (48) is also reproduced in the expansion up to terms of order $\widetilde{U}^2$. Since eqs. (43) is asymptotically exact, the higher-order terms in $\widetilde{U}$ do not change the low-energy behavior in eq. (56).

Note that eq. (56) follows from the fact that we have used $f_{\rm eff}(\omega)$ for the distribution function of the free quasiparticles. This assumption seems to be justified also from the fact that the many-body effects on the correlated dis-

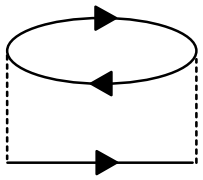

Fig. 5. The second-order diagram of $\widetilde{\boldsymbol{\Sigma}}$. The dashed represents $\widetilde{U}$, and solid lined represents the free-quasiparticle propagator $\widetilde{\boldsymbol{G}}_0$.

tribution $f^U_{\rm eff}(\omega)$ defined in eq. (20) arise first in the order U^2 contribution.

4.2 Beyond the Fermi-liquid regime

To study the higher-energy behavior at large ω, T, and eV with the RPT, one needs to calculate the higher order terms in $\widetilde{U}$. In the following, we describe the outline of the procedure of the expansion.

At high energies the renormalization factor z cannot be defined with respect to $T=0$ and $eV=0$ no longer. This is because the coefficient of the ω-linear term of the self-energy depends on T and eV. For instance, in the next order, the terms of the form $T^2\omega$ and $(eV)^2\omega$ exist. Therefore, z is redefined such that the ω-linear contributions in eq. (55) cancel out

$$\left.\frac{\partial\widetilde{\Sigma}^r(\omega)}{\partial\omega}\right|_{\omega=0} = 0\,. \tag{57}$$

Hence z generally depends on T and eV. The perturbation expansion in $\widetilde{U}$ can be carried out following that in the equilibrium case.[25] We first of all rewrite the action S in the form

$$S = z^{-1}\widetilde{S}_0 + z^{-2}S_U\widetilde{U}/U - S_{\rm cou} \tag{58}$$

$$S_{\rm cou} = \lambda\, z^{-2}S_U\widetilde{U}/U + z^{-1}\widetilde{S}_0 - S_0\,, \tag{59}$$

where $\widetilde{S}_0$ is the action for the free quasiparticle corresponding to the propagator $\widetilde{\boldsymbol{G}}_0(\omega)$, and $\lambda\equiv 1-z^2U/\widetilde{U}$. In eqs. (58) and (59) the factor $1/U$ is introduced just to cancel the bare Coulomb interaction U included in S_U by the definition in eq. (28). The perturbation series in $\widetilde{U}$ is generated by taking $z^{-1}\widetilde{S}_0$ in eq. (58) to be the unperturbed part and taking the remaining terms $z^{-2}S_U\widetilde{U}/U - S_{\rm cou}$ to be the perturbed part. Here, $S_{\rm cou}$ is the counter-term which avoids overcounting of the many-body effects. Specifically, the last two terms in the right-hand side of eq. (59), which can be rewritten in the form

$$z^{-1}\widetilde{S}_0 - S_0 = \bigl(z^{-1}-1\bigr)\sum_\sigma\int_{-\infty}^{\infty}{\rm d}\omega\,\boldsymbol{\eta}^\dagger_\sigma(\omega)\boldsymbol{\tau}_3\,\omega\,\boldsymbol{\eta}_\sigma(\omega)\,. \tag{60}$$

It corresponds to the counter-term for the renormalization factor z. In the RPT, the two parameters z and λ are regarded as functions of the renormalized parameters $\widetilde{\Delta}$ and $\widetilde{U}$, and are expanded as series in the powers of $\widetilde{U}$. Then the expansion coefficients for z and λ can be determined such that the two renormalization conditions, eqs. (57) and (61), are satisfied by each order in $\widetilde{U}$;

$$\widetilde{\Gamma}_{\uparrow\downarrow;\downarrow\uparrow}(0,0;0,0) = \widetilde{U}\,. \tag{61}$$

Here $\widetilde{\Gamma}_{\uparrow\downarrow;\downarrow\uparrow}\equiv z^2\Gamma_{\uparrow\downarrow;\downarrow\uparrow}$ is the vertex part for the four external causal Green's functions $\widetilde{G}^{--}$. In the RPT, $\widetilde{\Gamma}_{\uparrow\downarrow;\downarrow\uparrow}(0,0;0,0)$ is calculated in the power series in $\widetilde{U}$, and at high-energies it generally depends on T and eV. Note that the contribution of the parameter λ first arises in the order $\widetilde{U}^3$ terms.[25] For this reason, the condition of λ is not necessary to be taken into account in the expansion up to order $\widetilde{U}^2$.

As already mentioned, higher-order terms in $\widetilde{U}$ are needed to study the high-energy behavior of $\widetilde{\Sigma}^r(\omega)$ and dI/dV beyond the ω^2- and $(eV)^2$-terms. One possibility is to include the contributions up to terms of order $\widetilde{U}^4$. The corresponding calculations in the bare-U expansion have been carried out by Fujii and Ueda.[24] Alternatively, in the equilibrium case at $eV=0$, a combination of the RPT and NRG has been examined recently, and the results reproduce the T-dependence of the spin susceptibility accurately in a wide temperature range.[26] Such a combination would be another possibility to go beyond the Fermi-liquid regime at large bias voltages.

5. Summary

We have studied the low-energy properties of the Anderson model under a finite bias voltage V using the properties of the Keldysh Green's function at the impurity site $\boldsymbol{G}(\omega)$ as a functional of the nonequilibrium distribution function $f_{\rm eff}(\omega)$. Through the distribution function $f_{\rm eff}(\omega)$, the T- and eV-dependence of $\boldsymbol{G}(\omega)$ arise. The Ward identities for the derivative of the self-energy with respect to eV follow from these properties that can be summarized in the form of eq. (30). Using the Ward identities, the differential conductance dI/dV has been determined up to terms of order $(eV)^2$ in eq. (48) in the electron-hole symmetric case. The coefficients are determined by two characteristic parameters $\widetilde{\Delta}$ and R.

We have also described the low-energy properties using the renormalized perturbation theory in the Keldysh formalism. To second order in $\widetilde{U}$, it reproduces the exact $(eV)^2$ coefficients for dI/dV. The Fermi-liquid behavior of dI/dV follows from the assumption that the distribution function for the free quasiparticles are the same as that of the noninteracting electrons $f_{\rm eff}(\omega)$. In order to study the corrections to the Fermi liquid theory at large bias voltages with the RPT, one needs to calculate the higher order terms in $\widetilde{U}$.

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Appendix: Derivation of eqs. (33)–(34)

The first derivative of the self-energy with respect to eV can be written, using eq. (30), as

$$\left.\frac{\partial\boldsymbol{\Sigma}_\sigma(\omega)}{\partial(eV)}\right|_{eV=0} = \sum_{\nu\nu'\sigma'}\int_{-\infty}^{\infty}{\rm d}\omega'\,\frac{\delta\boldsymbol{\Sigma}_{{\rm eq},\sigma}(\omega)}{\delta G^{\nu\nu'}_{0:{\rm eq},\sigma'}(\omega')}\left.\frac{\partial G^{\nu\nu'}_{0\sigma'}(\omega')}{\partial(eV)}\right|_{eV=0}. \tag{A·1}$$

Similarly, the derivative of $\boldsymbol{\Sigma}_\sigma(\omega)$ with respect to ω at $eV=0$ is written in the form,

$$\left(\frac{\partial}{\partial\omega}+\frac{\partial}{\partial E_d}\right)\boldsymbol{\Sigma}_{{\rm eq},\sigma}(\omega) = \sum_{\nu\nu'\sigma'}\int_{-\infty}^{\infty}{\rm d}\omega'\,\frac{\delta\boldsymbol{\Sigma}_{{\rm eq},\sigma}(\omega)}{\delta G^{\nu\nu'}_{0:{\rm eq},\sigma'}(\omega'+\omega)} \times\left(\frac{\partial}{\partial\omega}+\frac{\partial}{\partial E_d}\right)G^{\nu\nu'}_{0:{\rm eq},\sigma'}(\omega'+\omega)$$

$$= \sum_{\nu\nu'\sigma'} \int_{-\infty}^{\infty} \mathrm{d}\omega' \frac{\delta \mathbf{\Sigma}_{\mathrm{eq},\sigma}(\omega)}{\delta G^{\nu\nu'}_{0:\mathrm{eq},\sigma'}(\omega')} \times \left(\frac{\partial}{\partial \omega'} + \frac{\partial}{\partial E_d} \right) G^{\nu\nu'}_{0:\mathrm{eq},\sigma'}(\omega'). \quad (\mathrm{A}\cdot 2)$$

Here we have used the property that the frequency ω' can be shifted to $\omega' + \omega$ without changing the result. This is because the value of the self-energy does not change if all the frequencies which are assigned to the Green's functions in a closed-loop diagram are shifted by the same amount. Therefore, substituting eq. (32) into eq. (A·1), we obtain eq. (33).

To calculate the second derivative, the variation of the self-energy $\delta \mathbf{\Sigma}_\sigma$ must be calculated up to terms of order $(\delta f_{\mathrm{eff}})^2$, and we find

$$\begin{aligned} &\left. \frac{\partial^2 \mathbf{\Sigma}_\sigma(\omega)}{\partial (eV)^2} \right|_{eV=0} \\ &= \sum_{\nu\nu'\sigma'} \int_{-\infty}^{\infty} \mathrm{d}\omega' \frac{\delta \mathbf{\Sigma}_{\mathrm{eq},\sigma}(\omega)}{\delta G^{\nu\nu'}_{0:\mathrm{eq},\sigma'}(\omega')} \left. \frac{\partial^2 G^{\nu\nu'}_{0\sigma'}(\omega')}{\partial (eV)^2} \right|_{eV=0} \\ &\quad + \sum_{\substack{\nu_1\nu_2,\sigma' \\ \nu_3\nu_4,\sigma''}} \int_{-\infty}^{\infty} \mathrm{d}\omega' \mathrm{d}\omega'' \frac{\delta^2 \mathbf{\Sigma}_{\mathrm{eq},\sigma}(\omega)}{\delta G^{\nu_1\nu_2}_{0:\mathrm{eq},\sigma'}(\omega') \delta G^{\nu_3\nu_4}_{0:\mathrm{eq},\sigma''}(\omega'')} \\ &\qquad \times \left. \frac{\partial G^{\nu_1\nu_2}_{0\sigma'}(\omega')}{\partial (eV)} \frac{\partial G^{\nu_3\nu_4}_{0\sigma''}(\omega'')}{\partial (eV)} \right|_{eV=0}. \end{aligned} \quad (\mathrm{A}\cdot 3)$$

Then flowing along the similar line, we obtain eq. (34) using eq. (32) and the corresponding relation for the second derivative

$$\left. \frac{\partial^2 G^{\nu\nu'}_0(\omega)}{\partial (eV)^2} \right|_{eV=0} = \kappa \left(\frac{\partial}{\partial \omega} + \frac{\partial}{\partial E_d} \right)^2 G^{\nu\nu'}_{0:\mathrm{eq}}(\omega) \,, \quad (\mathrm{A}\cdot 4)$$

where $\kappa \equiv (\alpha_L^2 \Gamma_L + \alpha_R^2 \Gamma_R)/(\Gamma_L + \Gamma_R)$.

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